NASA TECH BRIEF

Real Fluid Properties of Normal and Parahydrogen

The problem:

In numerically calculating the real fluid properties of normal and parahydrogen, phase boundaries must be defined precisely to provide mathematical consistency; good initial estimates must be made; functional definition of properties must remain mathematically and physically consistent; all the saturation functions should be available as analytical representations of region boundaries; and, in the vicinity of the critical region, the density calculation must be stabilized.

The solution:

A computer program, which calculates the real fluid properties of normal or parahydrogen, using a library of single function calls without initial estimates.

How it's done:

All property evaluations involving equations of state are preceded by a region-finding process to determine which equation of state applies.

While the region is directly specified by inputting temperature and density, indirect methods are used for region determination when only the combinations of pressure and density or of pressure and temperature are input. The region-finding process provides the additional information required to initiate iterations and to specify boundary values.

The evaluation of pressure is a direct substitution of the values of density and temperature in the appropriate state equation. Temperature and density procedures involve a method of successive approximations in which a sequence of trial values is generated by a Newton-type iteration.

To eliminate the stability problems of the density calculation in the vicinity of the critical region, two sets of density values are fit empirically for isotherms in the temperature range between 32.5° and 35°K. The variation of density with pressure in this region is then described by an interpolation formula. A modified Benedict–Webb–Rubin equation of state is used to calculate the values of pressure with the use of liquid or vapor coefficients. The result of this technique is a distortion of the vapor–liquid dome.

Given pressure and temperature, density is calculated, followed by enthalpy, entropy, specific heat, and viscosity; or temperature and density are calculated for a given value of pressure with enthalpy or entropy.

When only one parameter can be measured and a given phase value of the fluid is to be assumed, procedures are included to calculate saturated or ideal values of pressure and density as functions of temperature.

The library of property functions is used primarily for parahydrogen composition, however an option for normal hydrogen composition in the vapor region is included in the procedures for enthalpy, entropy, specific heat, and transport properties.

Notes:

1. This program is written in Fortran IV for use on the IBM 7094 computer.

2. Performance analysis of advanced propulsion systems, which use molecular hydrogen as both propellant and coolant, requires accurate knowledge of transport and thermodynamic properties in both the liquid and the vapor phase.

3. Inquiries concerning this program may be made to:
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   Computer Center
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   Reference: B68-10361

Patent status:
No patent action is contemplated by NASA.
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